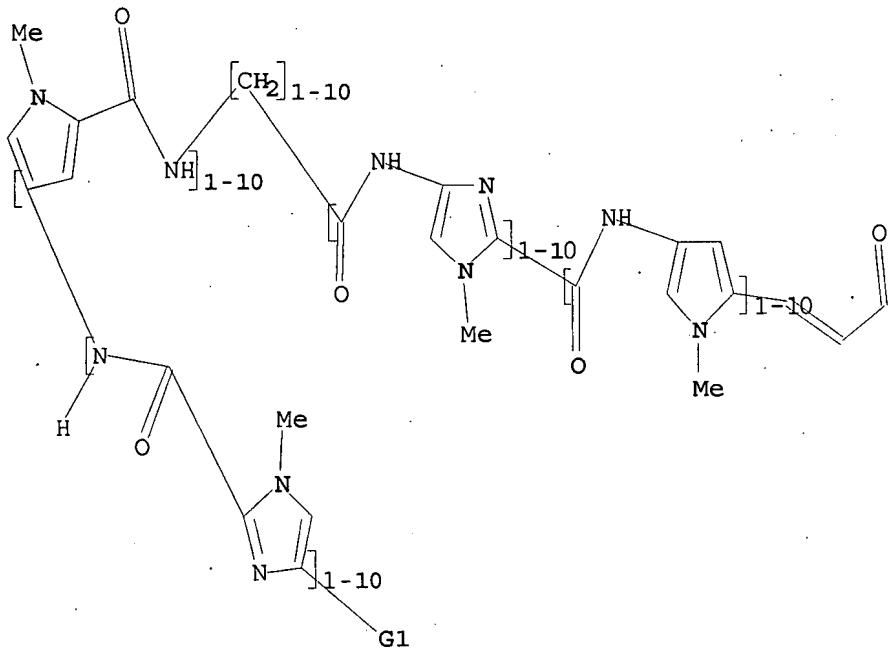
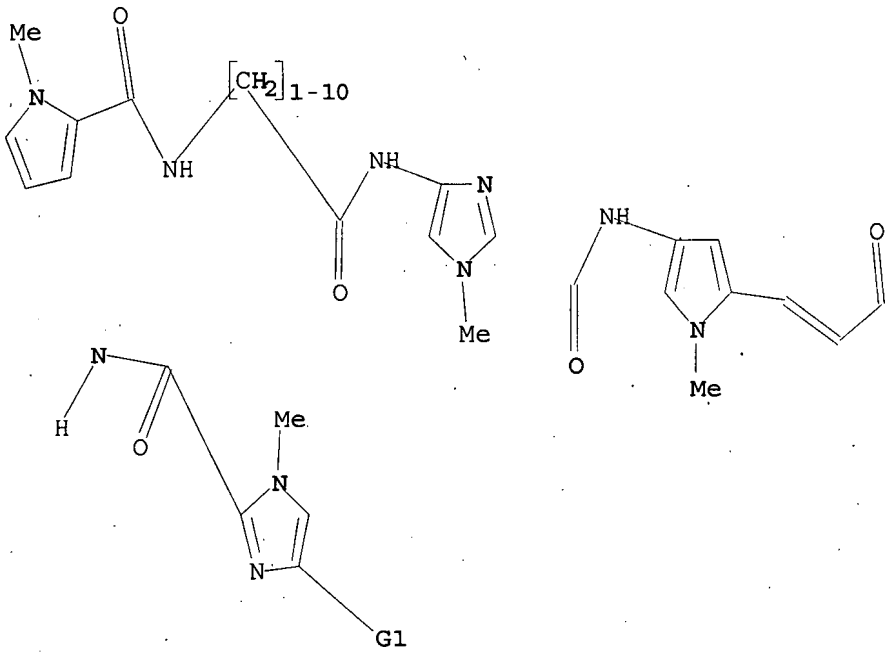
=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Ak,N

Structure attributes must be viewed using STN Express query preparation.

=> d l6
L6 HAS NO ANSWERS
L6 STR



G1 H,Ak,N

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 15:36:39 ON 24 JUL 2007)

FILE 'REGISTRY' ENTERED AT 15:37:11 ON 24 JUL 2007

L1		STRUCTURE UPLOADED
L2		QUE L1
L3	1	S IMIDAZOLE/CN
L4	1	S PYRROLE/CN
L5	132949	S 16.195/RID AND 16.136/RID
L6		STRUCTURE UPLOADED
L7		QUE L6
L8	0	S L6
L9	20	S L6 FUL
L10	20	S L9 AND CAPLUS/LC
L11	0	S L9 AND CAOLD/LC

FILE 'ZCAPLUS' ENTERED AT 15:43:19 ON 24 JUL 2007

L12	8	S L9

7/24/07

L12 ANSWER 8 OF 8 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:840303 ZCAPLUS <<LOGINID::20070724>>
DOCUMENT NUMBER: 138:132742
TITLE: Molecular design of a pyrrole - imidazole hairpin polyamides for effective DNA alkylation
AUTHOR(S): Bando, Toshikazu; Narita, Akihiko; Saito, Isao; Sugiyama, Hiroshi
CORPORATE SOURCE: Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, 101-0062, Japan
SOURCE: Chemistry--A European Journal (2002), 8(20), 4781-4790
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:132742

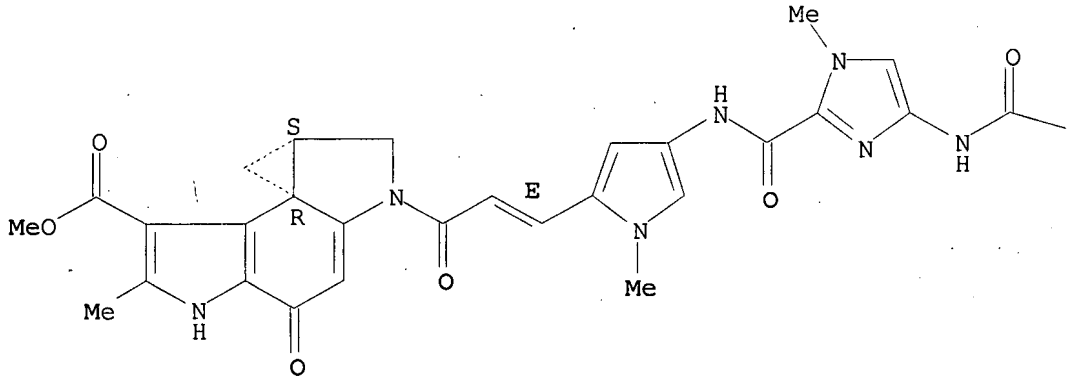
AB New hairpin polyamide-CPI (CPI = cyclopropylpyrroloindole) conjugates, compds. 12-14, were synthesized and their DNA-alkylating activities compared with the previously prepared hairpin polyamide, compound 1, by high-resolution denaturing gel electrophoresis with 450 base pair (bp) DNA fragments and by HPLC product anal. of the synthetic decanucleotide. In accord with our previous results, alkylation by compound 1 occurred predominantly at the G moiety of the sequence 5'-AGTCAG-3' (site 3). However, compound 12, in which the structure of the alkylating moiety of compound 1 is replaced with segment A of duocarmycin A DU-86 (CPI), did not show any DNA alkylating activity. In clear contrast, the hairpin CPI conjugate 13, which differs from compound 1 in that it lacks one Py unit and possesses a vinyl linker, alkylated the A of 5'-AGTCAG-3' (site 3) efficiently at nanomolar concns. Alkylation by compound 14, which has a vinyl linker, occurred at the A of 5'-AGTCCA-3' (site 6) and at several minor alkylation sites, including mismatch alkylation at A of 5'-TCACAA-3' (site 2). The significantly different reactivity of the alkylating hairpin polyamides 1, 12, 13, and 14 was further confirmed by HPLC product anal. by using a synthetic decanucleotide. The results suggest that hairpin polyamide-CPI conjugate 13 alkylates effectively according to Dervan's pairing rule, and with a new mode of recognition in which the Im-vinyl linker (L) pair targets G-C base pairs. These results demonstrate that incorporation of the vinyl-linker pairing with Im dramatically improves the reactivity of hairpin polyamide-CPI conjugates.

IT **491647-63-3P** **491647-64-4P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(vinyl-linker pairing with imidazole in pyrrole - imidazole hairpin can improve polyamides for effective DNA alkylation)

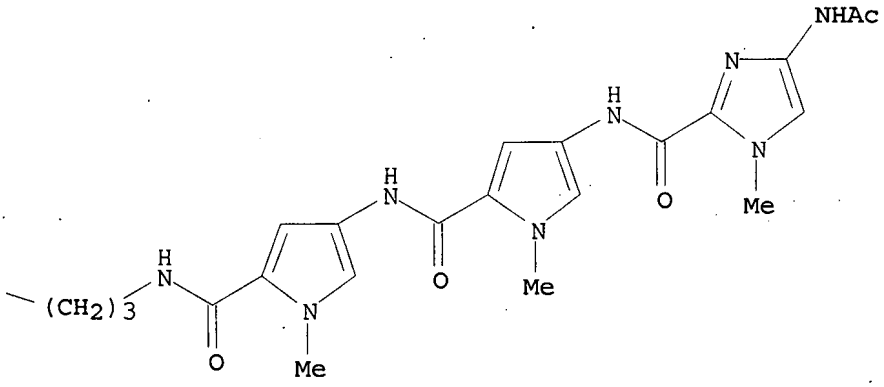
RN 491647-63-3 ZCAPLUS
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

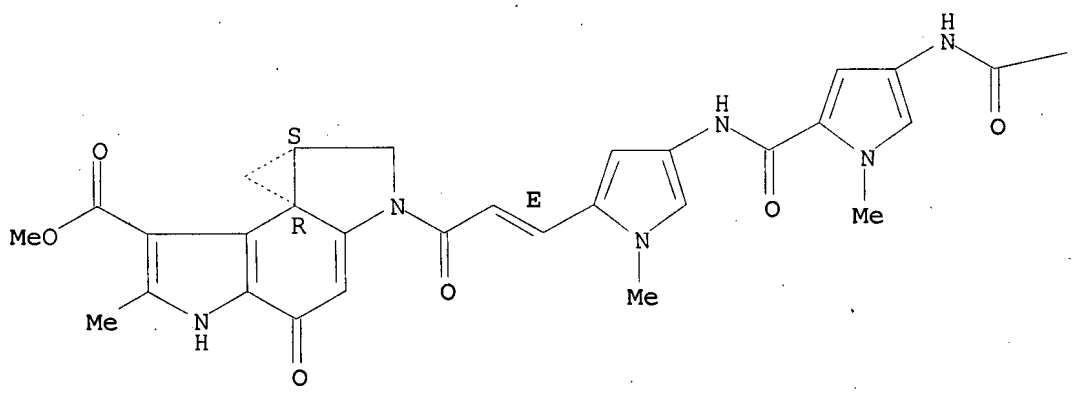


RN 491647-64-4 ZCAPLUS

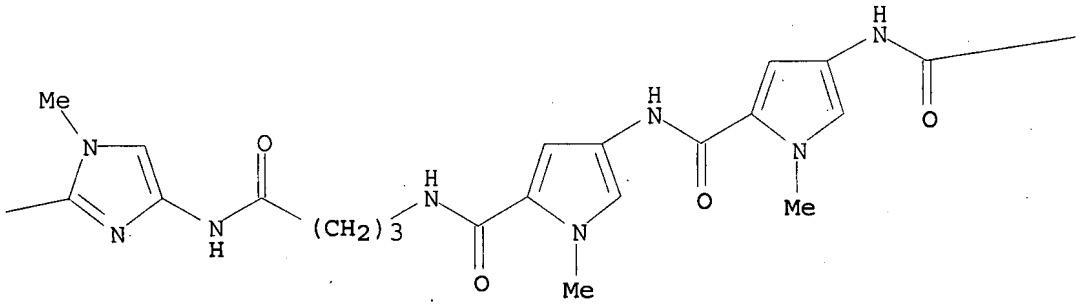
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

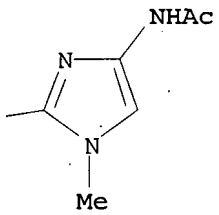
PAGE 1-A



PAGE 1-B



PAGE 1-C



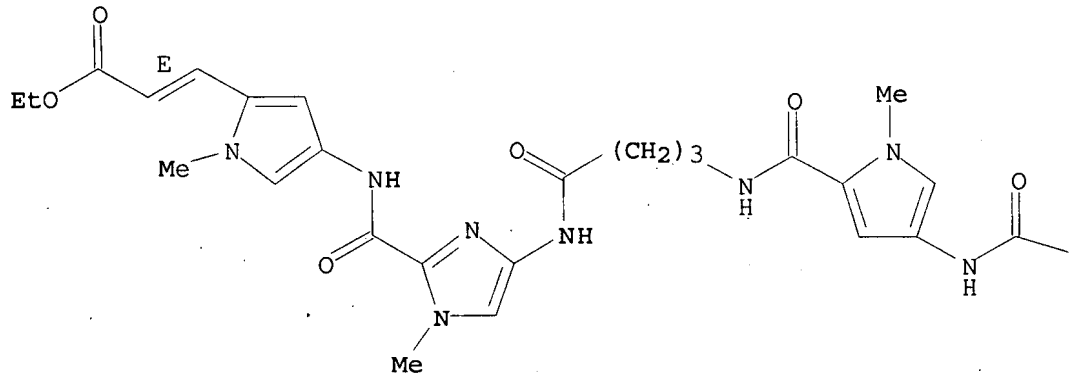
IT **491647-57-5P 491647-58-6P 491647-59-7P**
491647-60-0P 491647-61-1P 491647-62-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(vinyl-linker pairing with imidazole in pyrrole - imidazole hairpin can improve polyamides for effective DNA alkylation)

RN 491647-57-5 ZCAPLUS

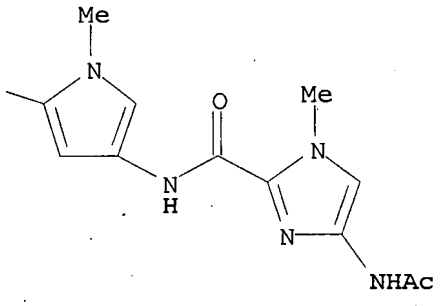
CN 2-Propenoic acid, 3-[4-[[[4-[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



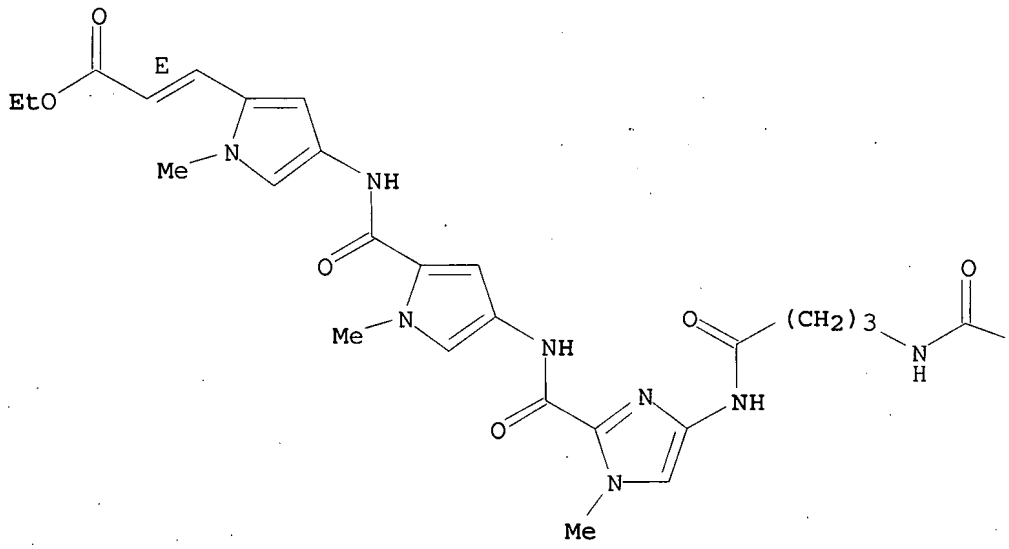
PAGE 1-B



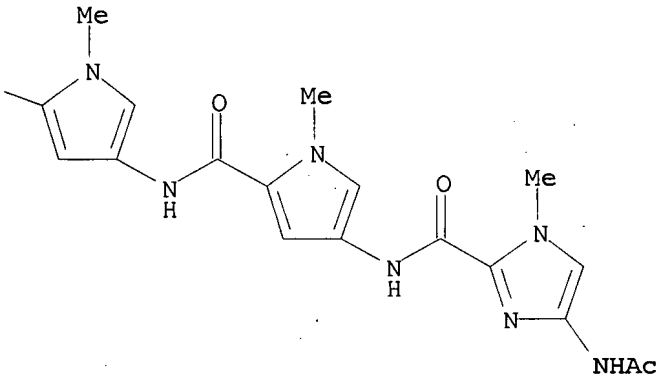
RN 491647-58-6 ZCAPLUS
CN 2-Propenoic acid, 3-[4-[[[4-[[[4-[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

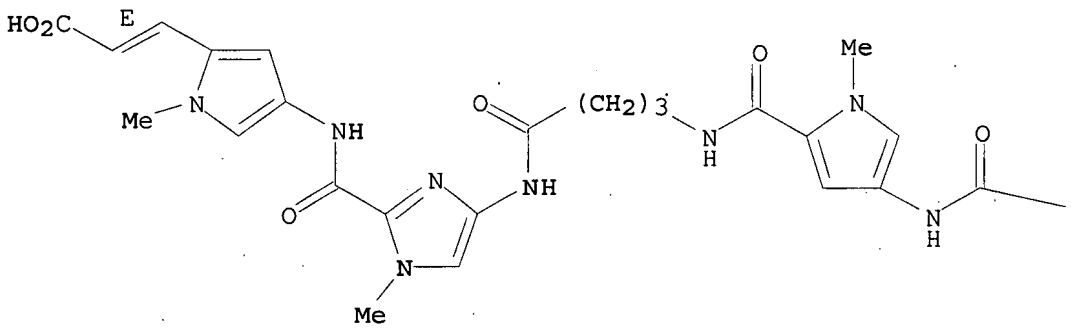


RN 491647-59-7 ZCAPLUS

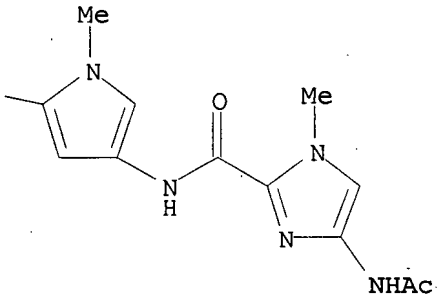
CN 2-Propenoic acid, 3-[4-[[[4-[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



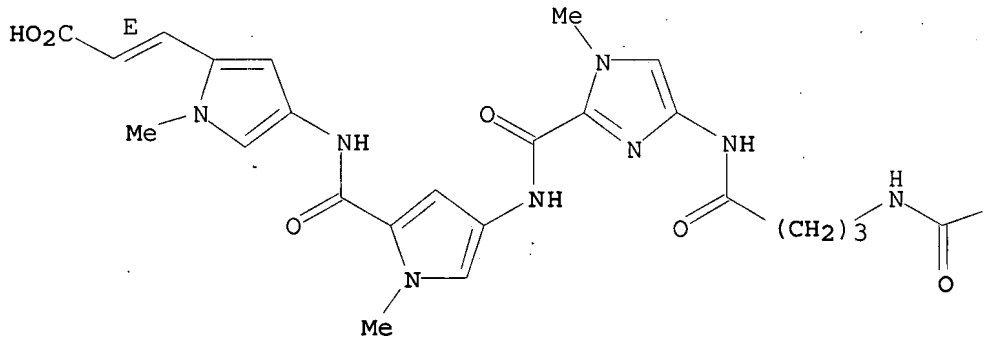
PAGE 1-B



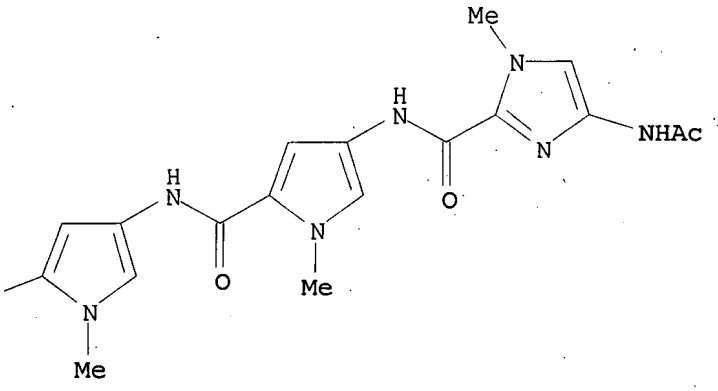
RN 491647-60-0 ZCAPLUS
CN 2-Propenoic acid, 3-[4-[[[4-[[[4-[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



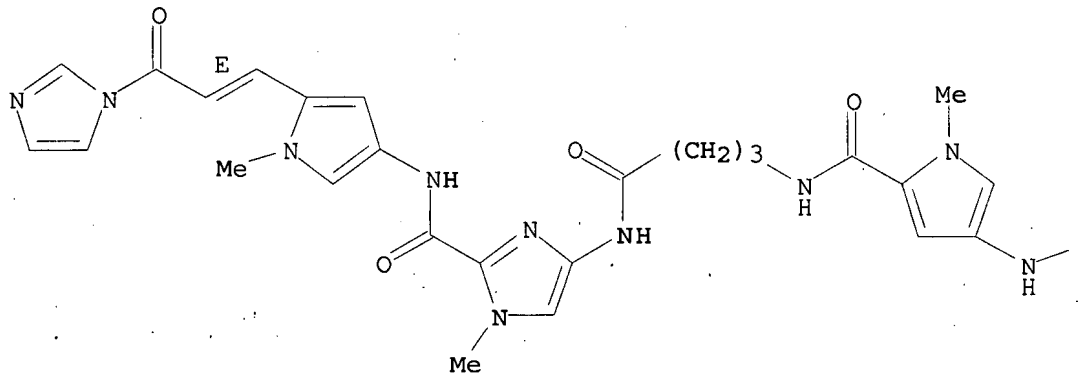
PAGE 1-B



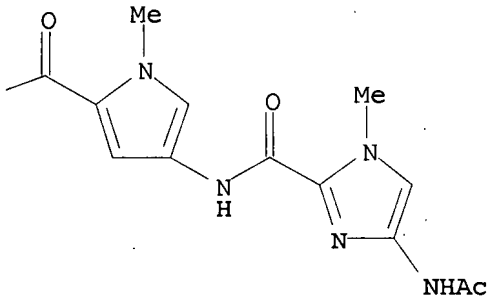
RN 491647-61-1 ZCAPLUS
CN 1H-Imidazole-2-carboxamide, 4-(acetylamino)-N-[5-[[[5-[[[4-[[2-[[[5-[(1E)-3-(1H-imidazol-1-yl)-3-oxo-1-propenyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]-4-oxobutyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

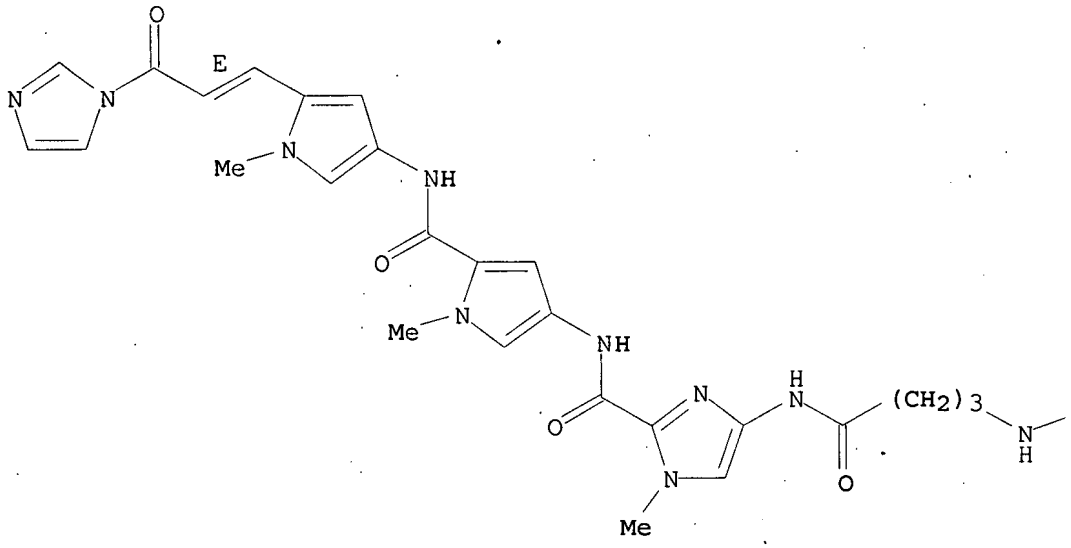


RN 491647-62-2 ZCAPLUS

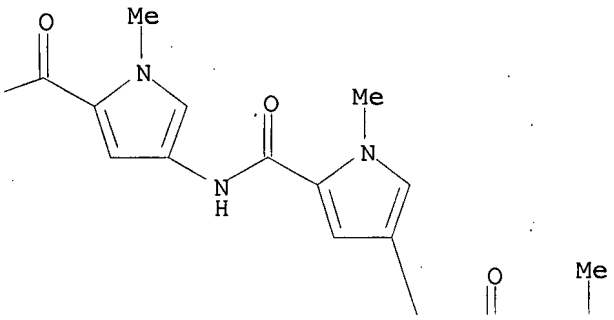
CN 1H-Imidazole-2-carboxamide, 4-(acetylamino)-N-[5-[[[5-[[[4-[[2-[[[5-[[[5-[(1E)-3-(1H-imidazol-1-yl)-3-oxo-1-propenyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]-4-oxobutyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



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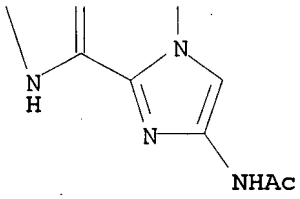

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT